

Numerical Modeling Study of CO₂ Storage in Brine Aquifer in Ferric Iron-Bearing Sandstone

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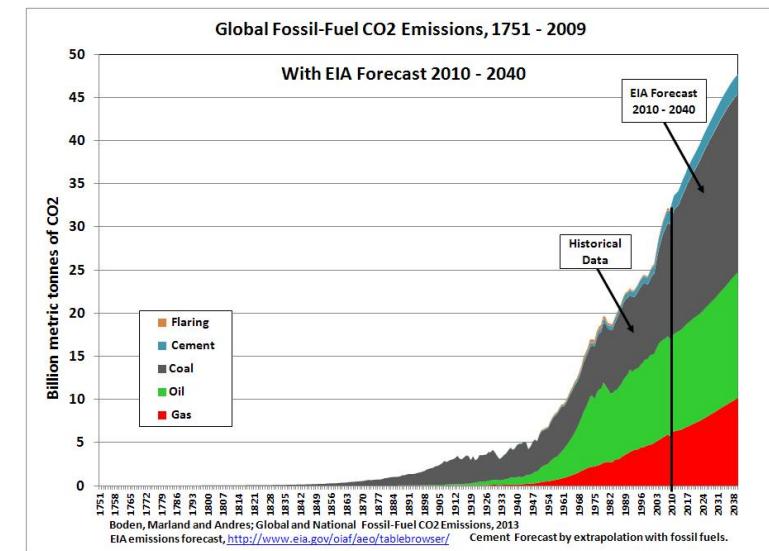
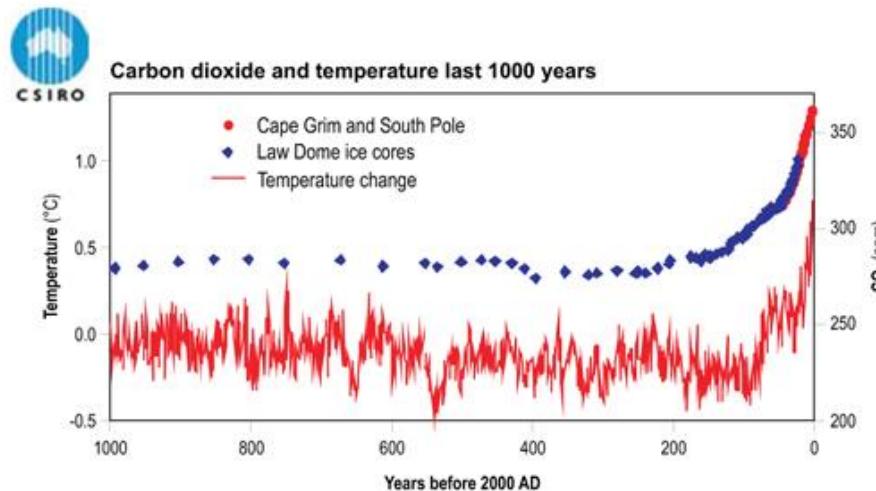
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Outline

- Background
- Core flooding experiment
- Simulations
- Results
- Summary

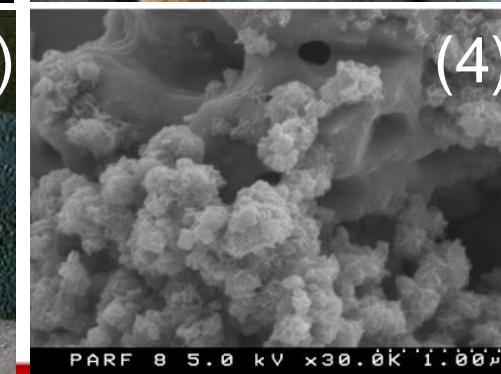
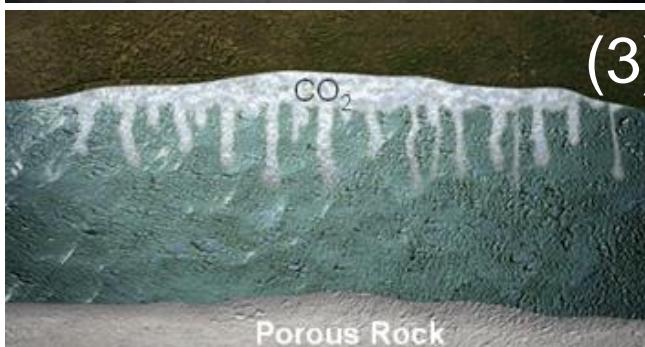
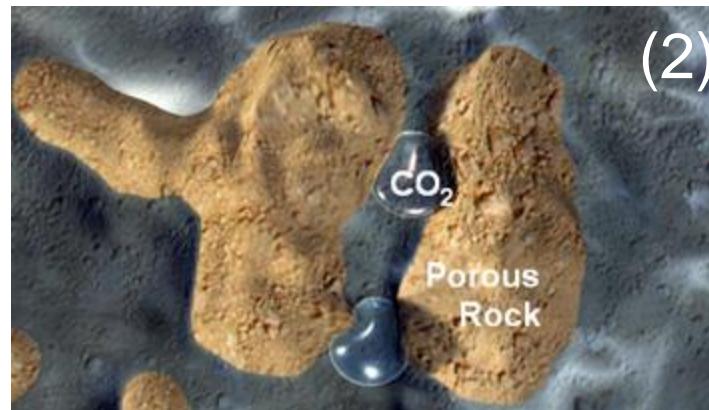
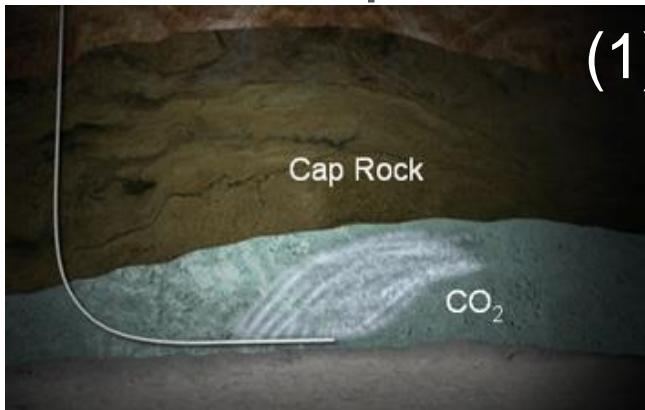
Background (1)

- Anthropogenic greenhouse emission and global warming effects



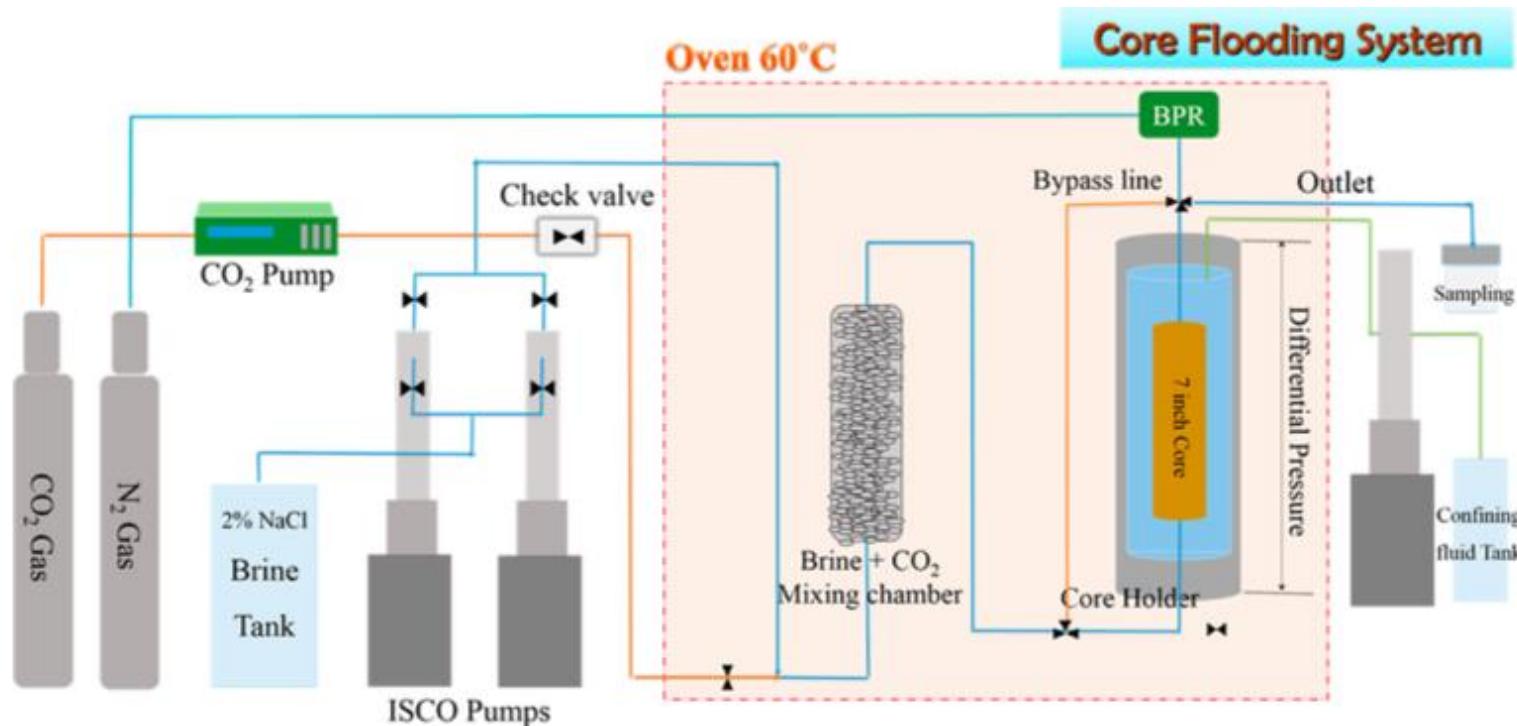
Background (2)

- Mechanisms of carbon sequestration in deep saline aquifers



- (1) Structural Trapping
- (2) Residual Trapping
- (3) Dissolution Trapping
- (4) Mineral Trapping

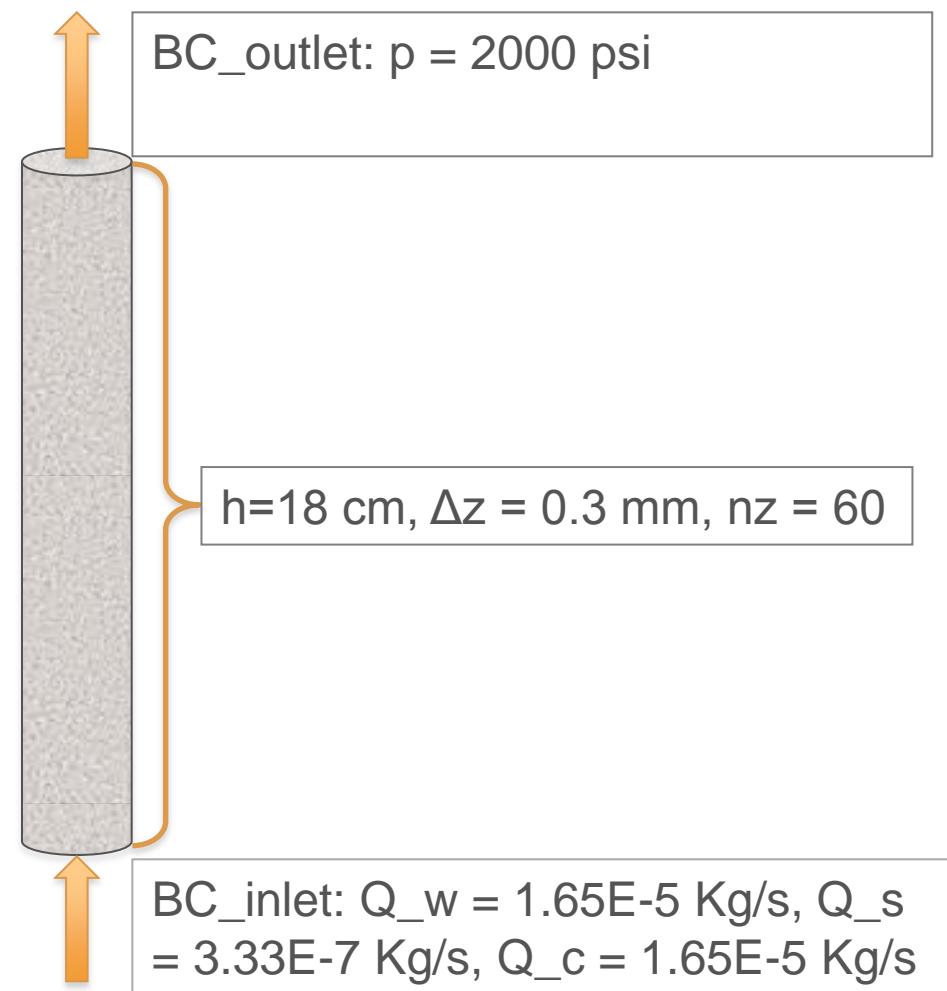
Core Flooding Experiment



Kwon, H., Payne, C., Deo, M. Reactive and Pore Structure Changes in Carbon Dioxide Sequestration. *Indus. & Eng. Chem. Research.* 2014, doi: 10.1021/ie503879a.

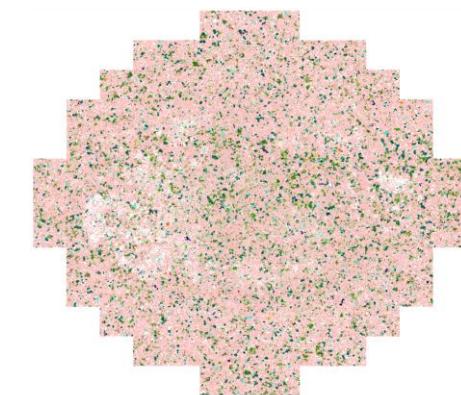
Simulations (1)

- TOUGHREACT with ECO2N EOS module
- 1D, homogeneous
- 2-phase, van Genuchten relative permeability and capillary pressure models



Simulations (2)

- Geochemical system
 - Minerals identified using QEMSCAN
 - Area fractions assumed to be volume fractions, total 96% accounted



	h2o	h+	ca+2	mg+2	na+	k+	fe+2	sio2(aq)	hco3-	alo2-	cl-
Quartz	0	0	0	0	0	0	0	1	0	0	0
K-feldspar	0	0	0	0	0	1	0	3	0	1	0
Illite	0.4	1.2	0	0.25	0	0.6	0	3.5	0	2.3	0
Kaolinite	1	2	0	0	0	0	0	2	0	2	0
Plagioclase	0	0	1	0	4	0	0	14	0	6	0
Smectites	0.52	0.96	0	0.26	0.29	0	0	3.97	0	1.77	0
Chlorite	8	-8	0	2.5	0	0	2.5	3	0	2	0
Siderite	0	-1	0	0	0	0	1	0	1	0	0
Ankerite	0	-2	1	0.3	0	0	0.7	0	2	0	0

Simulations (3)

- Reaction kinetics
 - Kinetic rate constants adjusted to match the experimental results
 - Surface area is representative for two groups: clay and non-clay minerals

	Initial volume Fraction (%)	Reactive Surface area (cm ² /g)	k ^{nu} (mol/m ² s)	k ^H (mol/m ² s)	k ^{OH} (mol/m ² s)
Quartz	60.85	9.8	1.02E-14		
K-feldspar	4.28	9.8	3.89E-13		
Illite	4.49	151.6	1.66E-13	1.05E-11	3.02E-17
Kaolinite	2.34	151.6	6.92E-14	4.90E-12	8.91E-18
Plagioclase	2.16	9.8	1.45E-13	2.14E-11	
Smectites	0.54	151.6	1.66E-13	1.05E-11	3.02E-17
Chlorite	0.65	9.8	3.02E-09	7.76E-12	
Siderite	0.08	9.8	1.26E-08	6.46E-04	
Ankerite	0.19	9.8	1.26E-09	6.46E-04	

Simulations (4)

- TST rate law

$$r_n = k_n A_n (1 - \Omega_n^\theta)^\eta \quad n = 1, \dots, N_q$$

$$\Omega_n = K_m^{-1} \prod c_i^v \gamma_i^v$$

$$\log K_m = a \ln T + b + cT + \frac{d}{T} + \frac{e}{T^2},$$

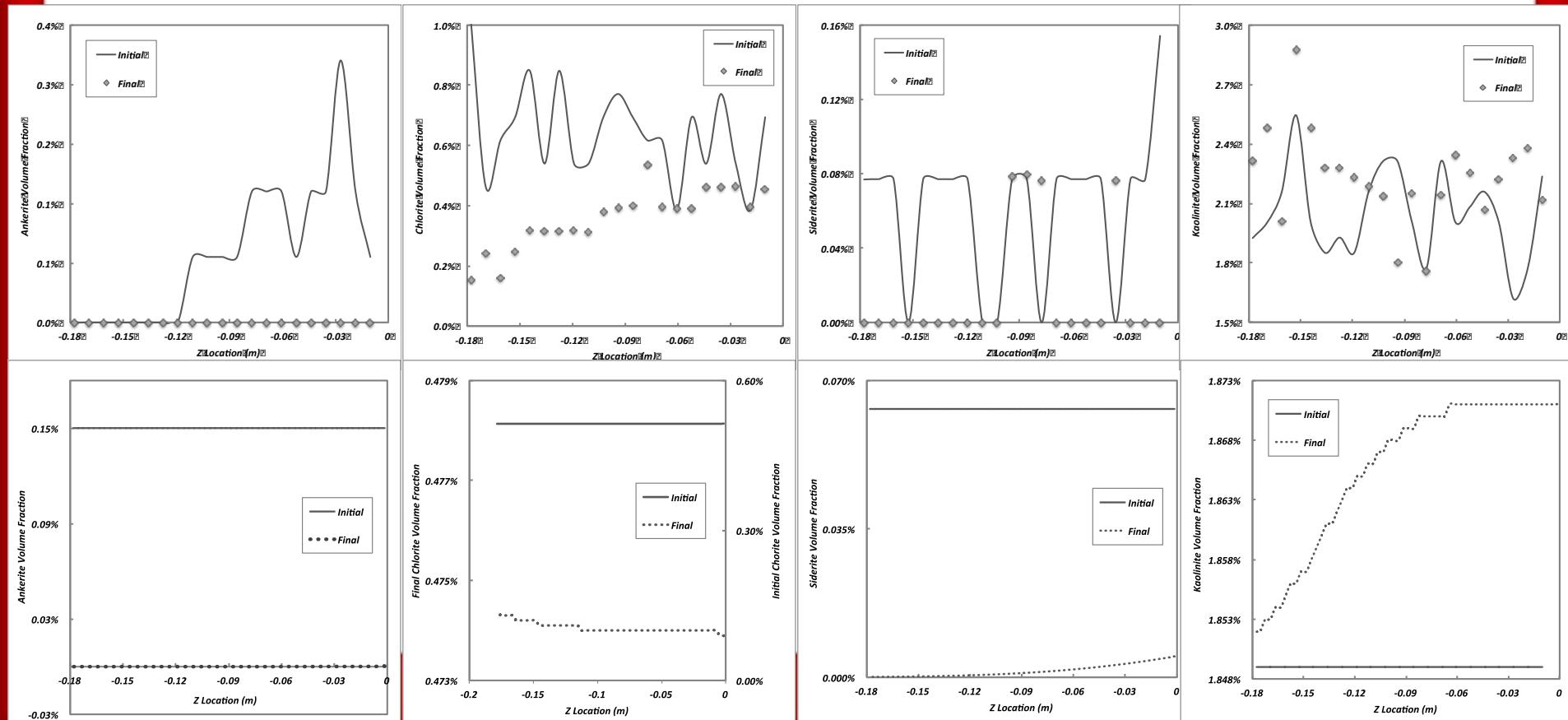
$$k = k_{25} \exp \left[\frac{-E_a}{R} \left(\frac{1}{T} - \frac{1}{298.15} \right) \right] + k_{25}^H \exp \left[\frac{-E_a^H}{R} \left(\frac{1}{T} - \frac{1}{298.15} \right) \right] a_H^{n_H} \\ + k_{25}^{OH} \exp \left[\frac{-E_a^{OH}}{R} \left(\frac{1}{T} - \frac{1}{298.15} \right) \right] a_{OH}^{n_{OH}}.$$

- Porosity-Permeability relationships

$$kp = kp_i (\phi / \phi_i)^3 \quad kp / kp_i = (1 - \phi_i)^2 / (1 - \phi)^2 \cdot (\phi / \phi_i)^3$$

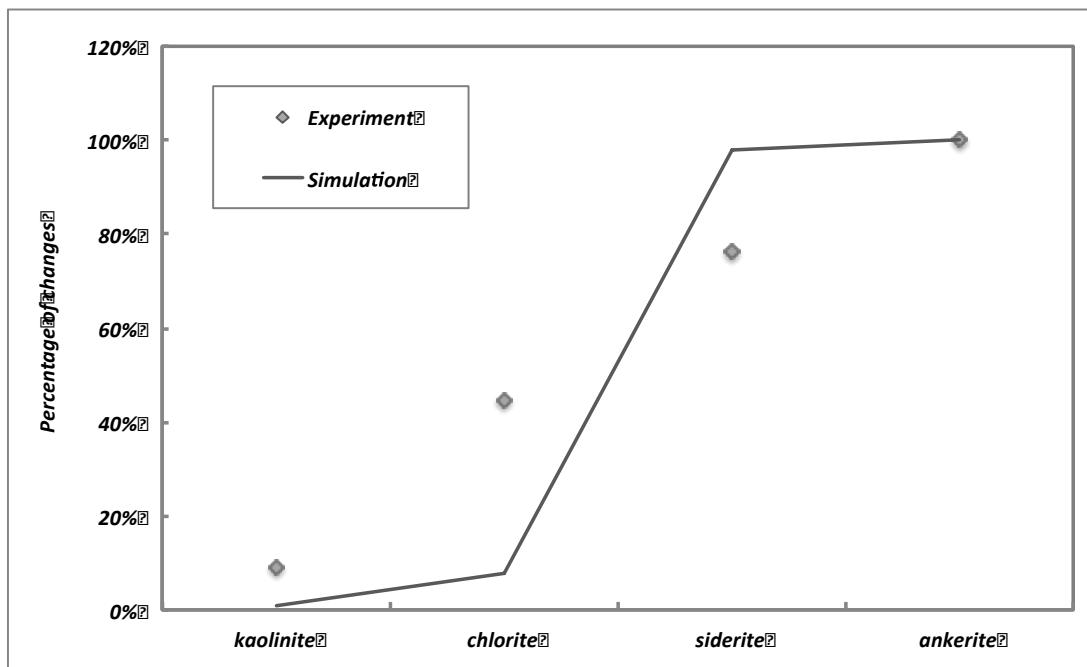
Results (1)

- Mineral distribution - dissolution dominant
 - Ankerite, Chlorite, Siderite, and Kaolinite



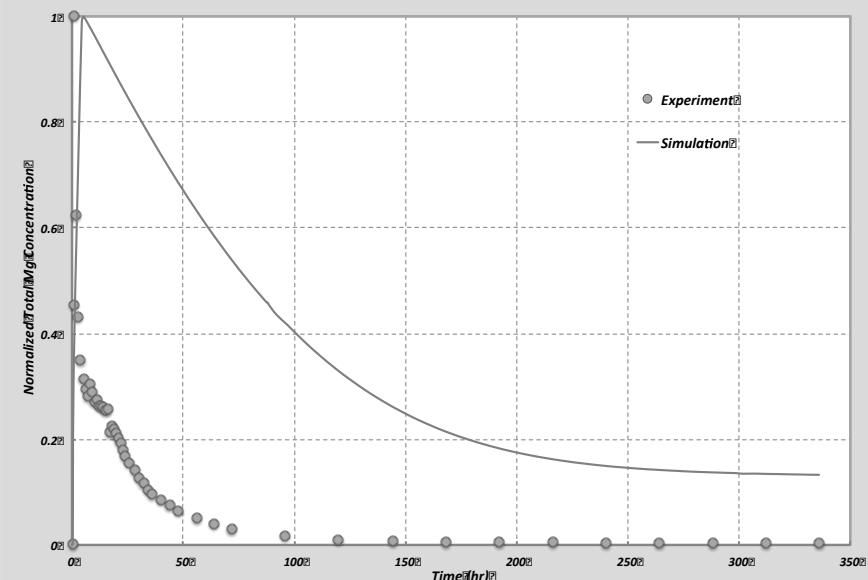
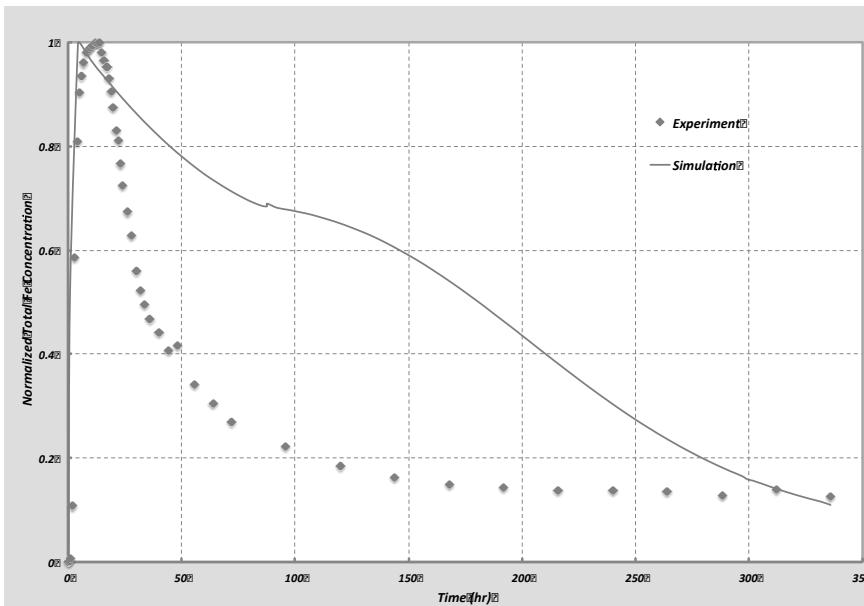
Results (2)

- Mineral distribution
 - Total relative changes



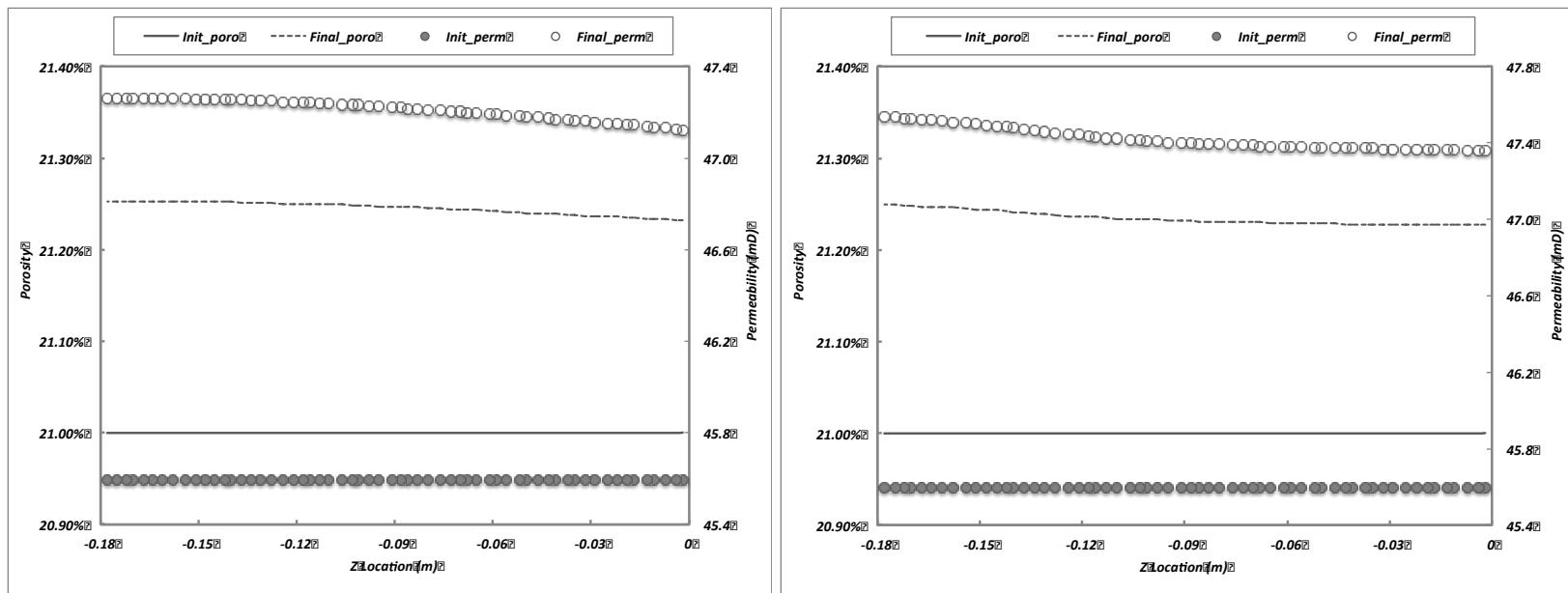
Results (3)

- Metal cation temporal evolution (Fe and Mg)
 - Discrepancy in absolute values
 - Normalized to compare trend



Results (4)

- Porosity and Permeability
 - Cubic law and Carman-Kozeny relationship
 - Max porosity 1.2% and permeability 5.1% max change



Summary

- At near wellbore scale where dissolution dominates, reactions take place faster than they do during storage.
- Mineral distribution is consistent with lab observations.
- High dissolved iron was observed. Temporal evolution trend can be captured, but discrepancy exists in the absolute values. Batch experiments will be carried out to accurately measure mineral kinetics.
- Compare to experiment, porosity and permeability is underestimated. May be subject to heterogeneity.

Acknowledgements

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Thank you! & Questions?